# Status of the R-matrix Code AMUR toward a consistent cross-section evaluation and covariance analysis for the light nuclei

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**Abstract.** We report the status of the R-matrix code AMUR toward consistent cross-section evaluation and covariance analysis for the light-mass nuclei. The applicable limit of the code is extended by including computational capability for the charged-particle elastic scattering cross-sections and the neutron capture cross-sections as example results are shown in the main texts. A simultaneous analysis is performed on the $^{17}$O compound system including the $^{16}$O($n,tot$) and $^{13}$C($\alpha,n$)$^{16}$O reactions together with the $^{16}$O($n,n$) and $^{13}$C($\alpha,\alpha$) scattering cross-sections. It is found that a large theoretical background is required for each reaction process to obtain a simultaneous fit with all the experimental cross-sections we analyzed. Also, the hard-sphere radii should be assumed to be different from the channel radii. Although these are technical approaches, we could learn roles and sources of the theoretical background in the standard R-matrix.

## 1. Introduction

The cross-sections on the light-nuclei are essential for nuclear science and engineering. The cross-sections are also drawing attention for the ion-beam analysis, the astrophysics and the medical applications. However, still inconsistencies exist between the measured and evaluated data, which could bring a large uncertainty in the practical applications. The R-matrix formalism [1] is rigorous and straightforward to the quantum mechanics, in which the S-matrix is deduced from the measured cross-sections in the resonance energy region. Furthermore, physical constraint from the theory is known as a big tool to reduce the problem arising from the differences among experimental data.

AMUR [2,3] is a multi-level and multi-channel R-matrix code which is being in progress towards a consistent cross-sections evaluation for the light-mass nuclei. We present the status of the code with new features on the theoretical calculation. This paper also focuses on the analysis of the $^{17}$O compound system, in which we technically solved a serious issue on the simultaneous fit of experimental cross-sections including those for the $^{13}$C($\alpha,\alpha$) elastic scattering.

## 2. Status of the AMUR code

### 2.1. Short summary of the code

AMUR is a multi-channel R-matrix code based on the Wigner and Eisenbud formalism [4]. Since the formalism is designed to obtain the S-matrix on a given boundary condition, both the cross-sections and the differential cross-sections are calculated with the code once we obtain resonance parameters such as the energy eigenvalue $E_\lambda$ and the reduced-width amplitude $\gamma_{\lambda c}$. Although the formalism itself is strictly based on the quantum mechanics, the only worrisome point is the use of the hard-sphere to calculate the phase-shifts of the shape-elastic scattering as we discuss later on.

Values of the resonance parameters are estimated from the experimental cross-sections with the generalized least-square method. The code is also designed to take account of the experimental resolution, renormalization and so on to obtain reasonable resonance parameters as much as possible. It should be noted that both the theoretical and experimental parameters could be obtained simultaneously, imposing the physical constraint from the theory effectively. Since the covariance of the resonance parameters are obtained from the measurements, covariance is also estimated for the cross-sections through the sensitivity matrix to the parameters. Such an approach is equivalent with the method in the KALMAN/SOK code [5].

### 2.2. Recent progress

The code was initially designed for the analysis of the incident neutrons as the evaluation of neutron cross-sections is in our most interest. However, the resonance parameters can be obtained from the experimental cross-section of the incident charged-particle if the reaction shares the same compound system. For example, the resonance parameter of the $^{17}$O system could be obtained not only from measurements for the n+$^{16}$O reactions but also from those for the $\alpha$+$^{13}$C reactions. Therefore, we incorporate the Coulomb-scattering amplitude to calculate the T-matrix elements, which enable us to analyze the charged-particle elastic-scattering differential cross-sections simultaneously with the other reactions. Example analysis with this option is presented in the next section.

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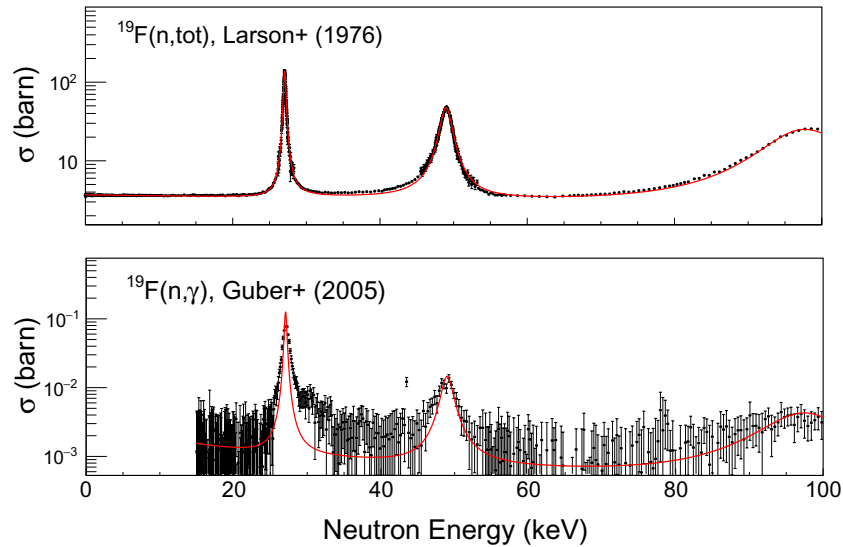[a] e-mail: `kunieda.satoshi@jaea.go.jp`

**Figure 1.** Preliminary results on the simultaneous analysis of measured neutron total cross-sections [7] and capture cross-sections [8] on $^{19}$F.

The neutron capture cross-sections are relevant with the reactor engineering and astrophysics. For the light-mass nuclei, the cross-sections are quite smaller than those for the heavier nuclei. However, we decided to incorporate a computational method into the code to achieve a consistent data evaluation. This is also essential to extend the applicable limit of the analysis toward the heavier-mass nuclei in the future. As a first step for the calculation, we incorporate the Rich-Moore approximation to the standard R-matrix theory as follows [6],

$$R_{cc'} = \sum_\lambda \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E - i\Gamma_{\lambda\gamma}/2}, \qquad (1)$$

and

$$\sigma_{capt.} = \sigma_{total} - \sum_{c' \notin \gamma} \sigma_{cc'}, \qquad (2)$$

where the parameter $\Gamma_{\lambda\gamma}$ denotes the total width for the capture reaction. Although the calculated S-matrix is not unitary anymore, we decided to use this option since the computational approach is quite simple as the capture cross-section is calculated by subtracting the sum of the other reactions from the total cross-section. Figure 1 illustrates preliminary results on the simultaneous analysis of measured neutron total cross-sections [7] and capture cross-sections [8] on $^{19}$F. Although the experimental conditions are not considered in this preliminary analysis, the fitted curves obtained are good enough to see an applicability of the calculational method.

# 3. Progress in analysis of the $^{17}$O compound system

## 3.1. Summary of our previous analysis

For evaluation of the n+$^{16}$O cross-section in a resonant energy region, we had performed an R-matrix analysis on the $^{17}$O system which had already been reported elsewhere [2,3]. Indeed, we obtained reasonable resonance parameters up to $E_n \sim 6\,$MeV through the simultaneous analysis of measured $^{16}$O($n,tot$), $^{13}$C($\alpha,n$) cross-sections. The substantial feature of the analysis was that we always assumed a re-normalization parameter for each measurement. Owing to the unitarity-constraint from the theory, such a re-normalization parameter was obtained with very small uncertainty. For example, the uncertainty obtained was always less than 0.5% while 3–5% systematic uncertainty was usually suggested by experimentalists. Such a constraint is useful especially when there exist large differences among the experimental data. Indeed, ∼30% difference is observed between the experimental data of Bair and Haas [9] and Harissopulos et al. [10]. Our shape analysis finally supported the former data, which was consistent with the preceding study by Hale et al. [11].

## 3.2. Problem in the analysis of $^{13}$C($\alpha, \alpha$) cross-sections and a possible solution

We did successfully fit measured cross-sections on the $^{16}$O($n, tot$) and $^{13}$C($\alpha, n$)$^{16}$O reactions, simultaneously. Reasonable fits are also obtained in the angular distribution for the $^{16}$O($n, n$) scattering. However, serious discrepancies were observed between the experimental $^{13}$C($\alpha, \alpha$) differential cross-sections of Heil et al. [12] and the R-matrix calculation with resonance parameters obtained in our previous analysis. This situation is illustrated in Fig. 2 with the dashed curves, where the calculated results seriously overestimate the experimental data at all the scattering angles except for the forward case. That is very strange since all the reactions share the same compound system $^{17}$O. It is also because we did not find such a problem in the analysis of $^{16}$O($n, n$) differential cross-sections (note that Coulomb-scattering amplitude is considered for the charged-particle elastic scattering).

Through a number of simultaneous analyses for those above reactions, we finally found an approach which "technically" solves the present issue. Indeed, we need two "tricks" on the standard R-matrix theory. One is additional theoretical-backgrounds which should be given only for each elastic scattering process. Hence the
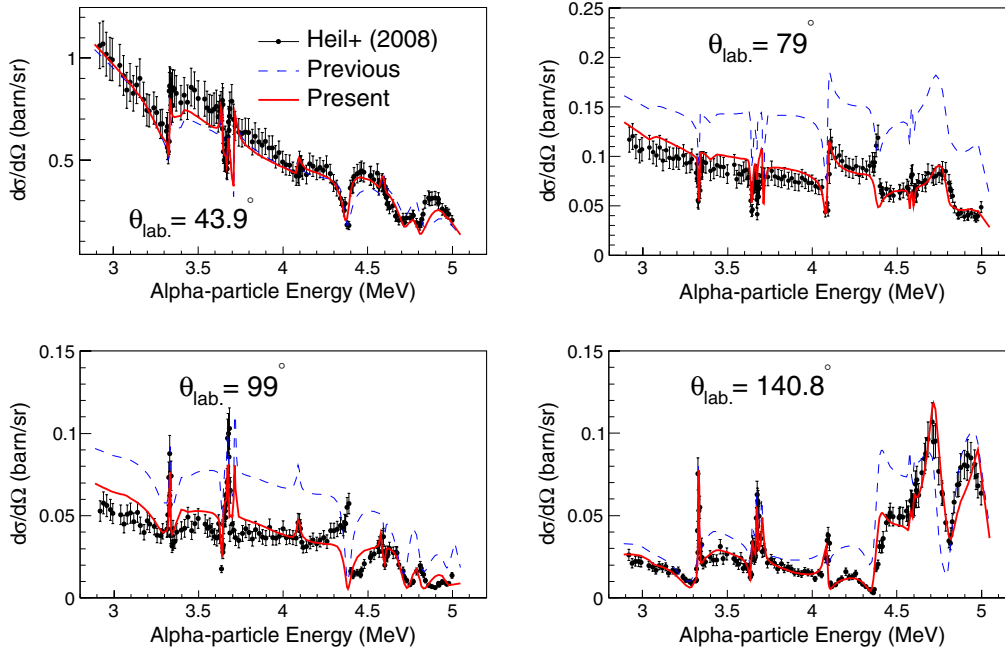
**Figure 2.** Calculated $^{13}C(\alpha, \alpha)$ differential cross-sections compared with the measured data of Heil et al [12]. The previous and present curves stand for the calculations from R-matrix analyses with and without the present approach described in the text, respectively.

**Table 1.** Values of the channel and hard-sphere radii obtained in the present analysis.

|  | $r_c$ (fm) | $r_\phi$ (fm) |
|---|---|---|
| n+$^{16}$O | 4.66 | 4.34 |
| $\alpha$+$^{13}$C | 6.90 | 5.55 |

R-matrix elements are calculated as follows,

$$R_{cc'} = \sum_\lambda \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E - i\Gamma_{\lambda\gamma}/2} + R_\infty^{(dist.)} + R_\infty^{(n)} + R_\infty^{(\alpha)},$$

(3)

where the symbol $R_\infty^{(dist.)}$ stands for the tail from the real distant levels, which is always required to take into account the interference effect from the compound states above the upper energy limit of the analysis. Additional terms are the distant poles $R_\infty^{(n)}$ and $R_\infty^{(\alpha)}$ which are given as the backgrounds for neutron and alpha-particle channels, respectively. The second trick is on the values of the hard-sphere radii $r_\phi$ where we assumed they could be different from the value of the channel radii $r_c$. Preliminary obtained values in the simultaneous fit are listed in Table 1. It should be noted that the values are almost equal for the n+$^{16}$O channel while the values are somewhat different for the $\alpha$+$^{13}$C channel.

If both tricks are considered in the analysis, the problem is dramatically improved as plotted in Fig. 2 with solid curves.

We need to admit that the present approach is quite "technical (less physics)" as we always referred it to "trick". However, the present results may suggest something in the R-matrix theory which has not been fully discussed over the years. At least, the sources of the theoretical backgrounds are much clearer, i.e., the source is not only from the distant levels but also from the shape-elastic scattering. That is, additional distant poles work as a correction to the hard-sphere scattering phase-shift for neutron and alpha-particle, separately. With those results,

we could have a hypothesis that such tricks are equivalent with having a Woods-Saxon type nuclear potential in the R-matrix. Of course, we need the model approaches to verify the hypothesis.

## 4. Summary and outlook

An R-matrix code AMUR is currently under development towards a consistent cross-section evaluation for the light-mass nuclei. We extended the applicable limit of the code by including computational capability for the charged-particle elastic scattering cross-sections and the neutron capture cross-sections. Our previous analysis of the $^{17}$O system was shortly summarized pointing out an issue on the simultaneous analysis with the experimental $^{13}C(\alpha, \alpha)$ differential cross-sections. The problem was "technically" solved if the theoretical background was given for neutron and alpha-particle channels individually in addition to the contributions from the distant levels, where we also needed to assume values of the channel and hard-sphere radii are different substantially for the $\alpha$+$^{13}$C channel. Upon those results, we could have a hypothesis that such tricks are equivalent with having a Woods-Saxon type nuclear potential in the R-matrix theory. We plan to perform the nuclear model analysis (such as the optical model analysis) to verify the hypothesis.

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